

Comparative analysis of alternative spectral bands of CO₂ and O₂ for the sensing of CO₂ mixing ratios

Denis Pliutau, and Narasimha S. Prasad

NASA Langley Research Center, 5 N. Dryden St., MS 468, Hampton VA, 23681

ABSTRACT

We performed comparative studies to establish favorable spectral regions and measurement wavelength combinations in alternative bands of CO₂ and O₂, for the sensing of CO₂ mixing ratios (XCO₂) in missions such as ASCENDS. The analysis employed several simulation approaches including separate layers calculations based on pre-analyzed atmospheric data from the modern-era retrospective analysis for research and applications (MERRA), and the line-by-line radiative transfer model (LBLRTM) to obtain achievable accuracy estimates as a function of altitude and for the total path over an annual span of variations in atmospheric parameters. Separate layer error estimates also allowed investigation of the uncertainties in the weighting functions at varying altitudes and atmospheric conditions. The parameters influencing the measurement accuracy were analyzed independently and included temperature sensitivity, water vapor interferences, selection of favorable weighting functions, excitations wavelength stabilities and other factors. The results were used to identify favorable spectral regions and combinations of on / off line wavelengths leading to reductions in interferences and the improved total accuracy.

1. INTRODUCTION

Currently missions involving active sensing of atmospheric gas concentrations from space are being planned for a number of atmospheric gases.¹ One of the molecules of interest for such space-based measurements is the CO₂ being investigated under the Active Sensing of CO₂ Emissions over Nights Days and Seasons (ASCENDS) mission recommended by NRC Decadal Survey.² The required accuracy of 0.3% in column averaged CO₂ mixing ratio determination presents a number of hard to overcome spectroscopic and technological obstacles requiring careful planning and analysis for the desired accuracy to be achievable.

To address the needs in space lidar predictive analysis, we have been involved in the development of a modeling framework based on a number of satellite datasets to facilitate selection of optimal spectral excitation spectral regions and improved measurement methodologies. Originally we attempted to use a direct approach in our optimization calculations with separate calculation runs for each of the location and date/time specific points over annual observation time span and all surface coordinates which turned out to be not feasible due to the computation complexity.³ This approach would only be possible using super-computer facilities and computer clusters. To address this problem and develop a set of modeling tool suitable for desktop computer applications we have modified our original approach by implementing pre-analysis of the datasets to be used for subsequent usage in the lidar sensitivity analysis. Such approach has already been demonstrated for the annual global analysis of the temperature and pressure data fields and is now being further extended to the surface elevation and reflection presently using the ASTER and MODIS datasets.^{4,5} The methodology involving pre-analysis of the numerical datasets is useful for global annual lidar optimization calculations. For single lidar estimate calculations, however, web-based architecture is being evaluated by introducing a number of libraries facilitating web-based data access and lidar optimization calculations involving the usage of satellite data for surface and atmospheric parameters.⁶

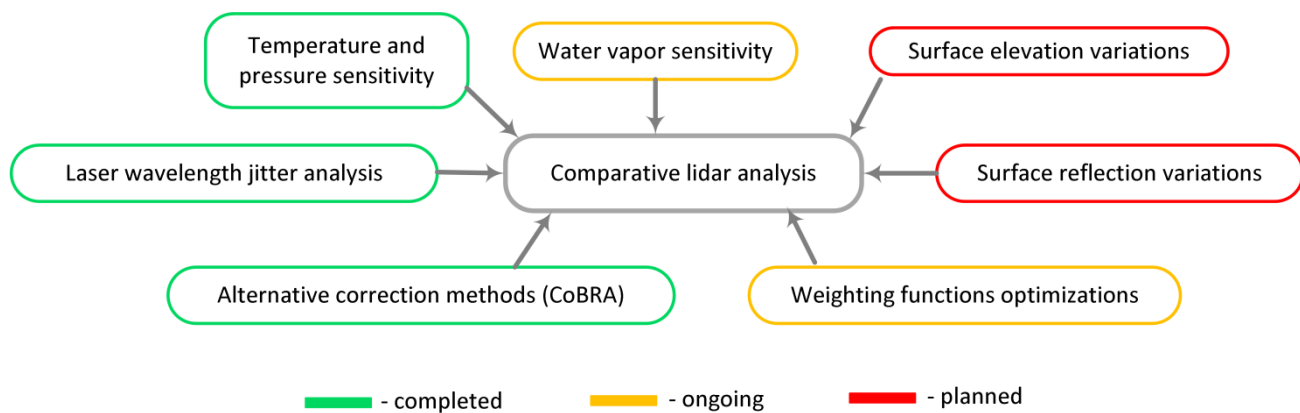


Fig 1. Illustration of the current state of the lidar simulation analysis components

The current state of our lidar analysis for the ASCENDS mission applications is summarized in Fig. 1. As can be seen multiple factors affecting accuracy have been considered for alternative bands of CO₂ and O₂ for the sensing of carbon dioxide concentrations with additional error reduction methodologies suggested. So far we have addressed the main sources of spectral variations such as temperature, pressure and wavelength stability effects with the exception of the surface elevation and reflection variations induced errors. The analysis of water vapor interferences is ongoing. The independent evaluation of all error components will enable the final selection of optimum excitation wavelengths and spectral bands to use for the lowest achievable error in the CO₂ mixing ratio measurements.

Previously we have performed laser wavelength jitter effects analysis for ASCENDS candidate bands of CO₂ and O₂ and also applied our modeling methodology to suggest an alternative CoBRA measurement approach for the molecular mixing ratio determination addressing some of the limitations of the pure Integrated Path Differential Absorption (IPDA) methodology.^{4,7-9} In this paper we describe temperature and pressure sensitivity analysis results for the alternative spectral bands of CO₂ and O₂ being considered for application in the ASCENDS mission carried out using the modeling framework we have been developing.

2. SINGLE WAVELENGTH TEMPERATURE AND PRESSURE SENSITIVITY ANALYSIS

In this section we report the “pure” temperature sensitivity analysis results not employing off-line wavelengths. The combined temperature and pressure sensitivity analysis methodology employed here is based on the use of the pre-analyzed global meteorological data with subsequent line-by-line transmission calculations as described in ^{4, 8, and 9}. Such simplified methodology allows obtaining coefficients of variation which take into account both temperature and pressure variations over an annual span and all geographical locations. We have used this approach to establish regions in the CO₂ and O₂ bands of interest exhibiting the lowest temperature sensitivity thus leading to higher accuracy measurements. It should be noted that the single wavelength coefficient of variation is calculated from the standard deviation and the mean values over an annual span and all locations thus being a direct representation of a relative uncertainty to be expected in annual satellite measurements at selected wavelengths assuming no corrections for known meteorological parameters.

Fig 2 illustrates the magnitude of temperature induced uncertainties due to annual temperature variations in the 6300 – 6380 cm⁻¹ spectral region of CO₂. As can be seen from Fig 2b, two regions of low temperature sensitivity are identified in the vicinity of 6320 and 6370 cm⁻¹ regions. Similar analysis performed for the 2.05 μm band is presented in Fig. 2. As can be seen from Fig 2b, two regions of low temperature sensitivity exist in the spectral regions close to 4830 and 4880 cm⁻¹. The results for these CO₂ spectral bands are consistent with the previous studies by Menzies.¹⁰

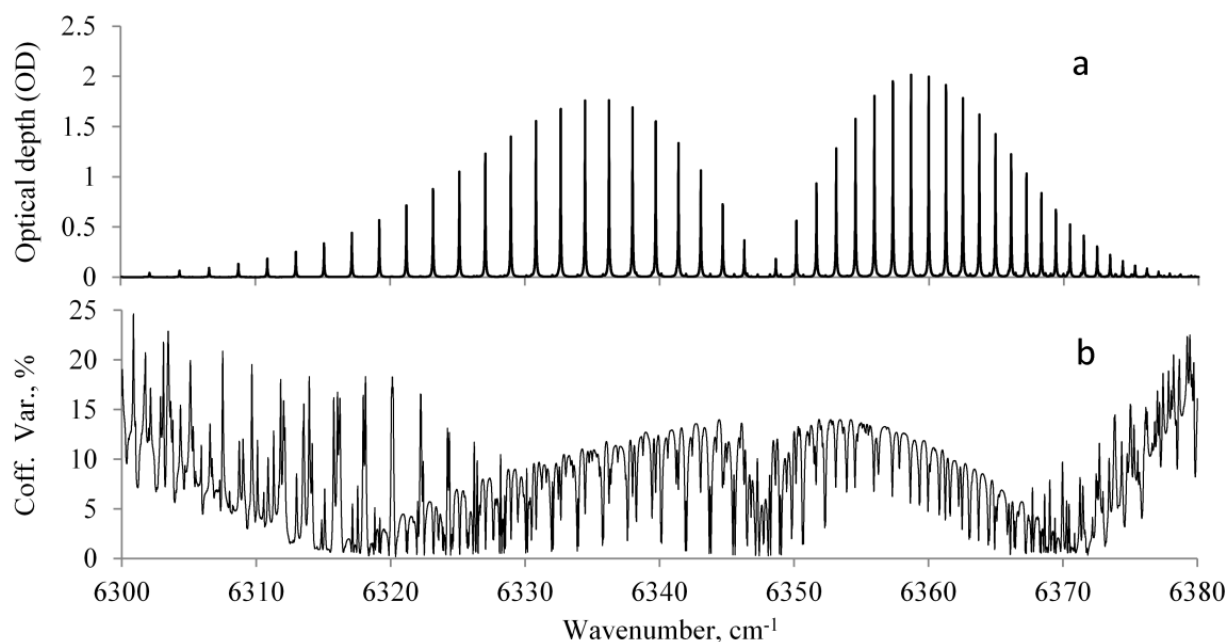


Fig 2 Total absorption spectrum (a) and the temperature induced error (b) for the 1.57 μm band of CO_2 due to annual variations in atmospheric temperature for year 2009.

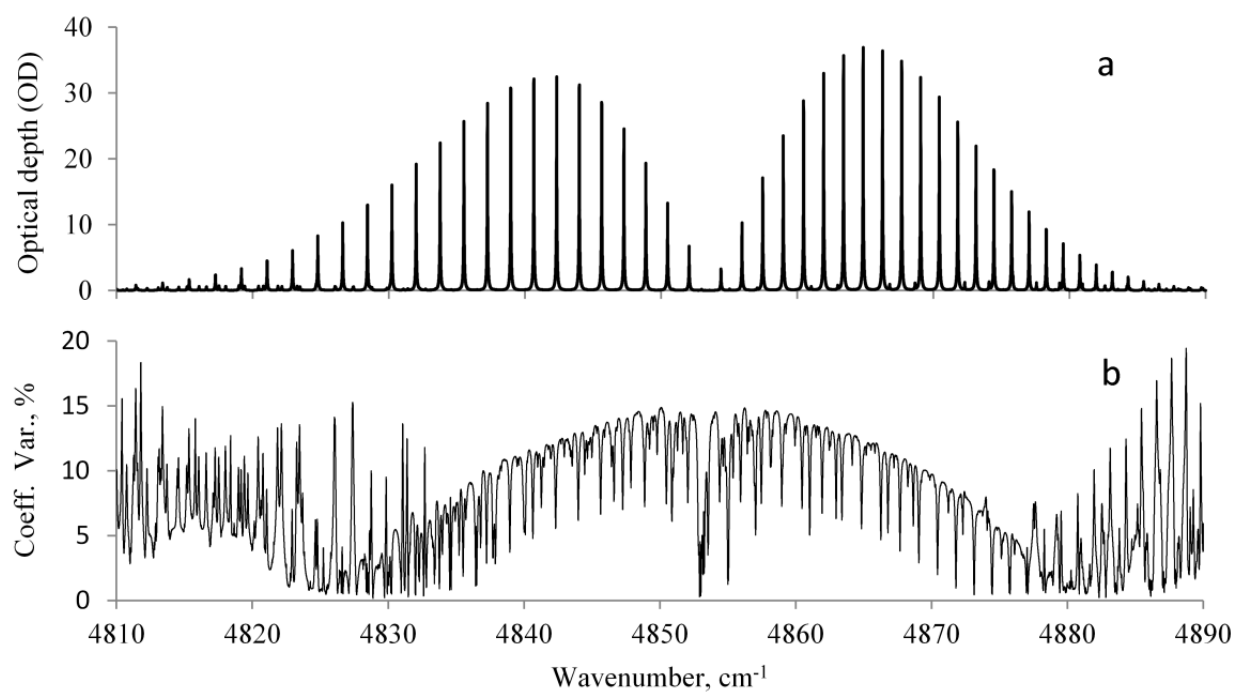


Fig 3. Total absorption spectrum for an 80km vertical path and US Standard atmospheric model (a) and the temperature induced error (b) for the 2.05 μm band of CO_2 due to annual variations in atmospheric temperature for year 2009.

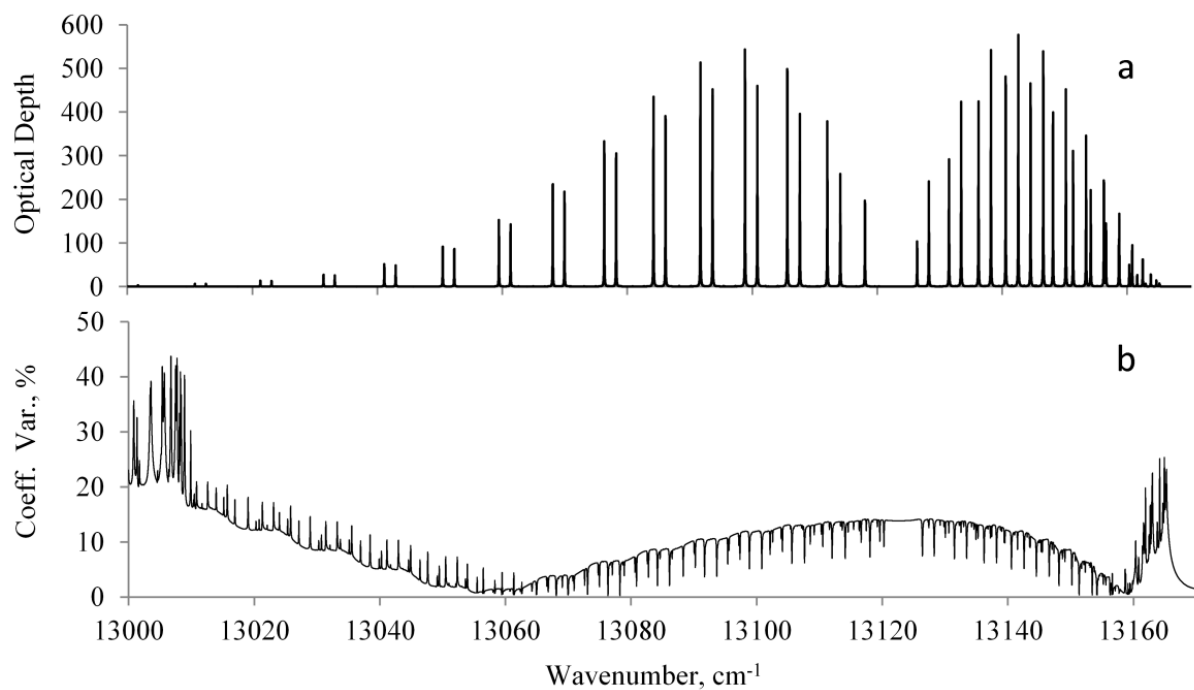


Fig 4. Total absorption spectrum for an 80km vertical path and US Standard atmospheric model (a) and the temperature induced error (b) for the A-Band band of O_2 due to annual variations in atmospheric temperature for year 2009.

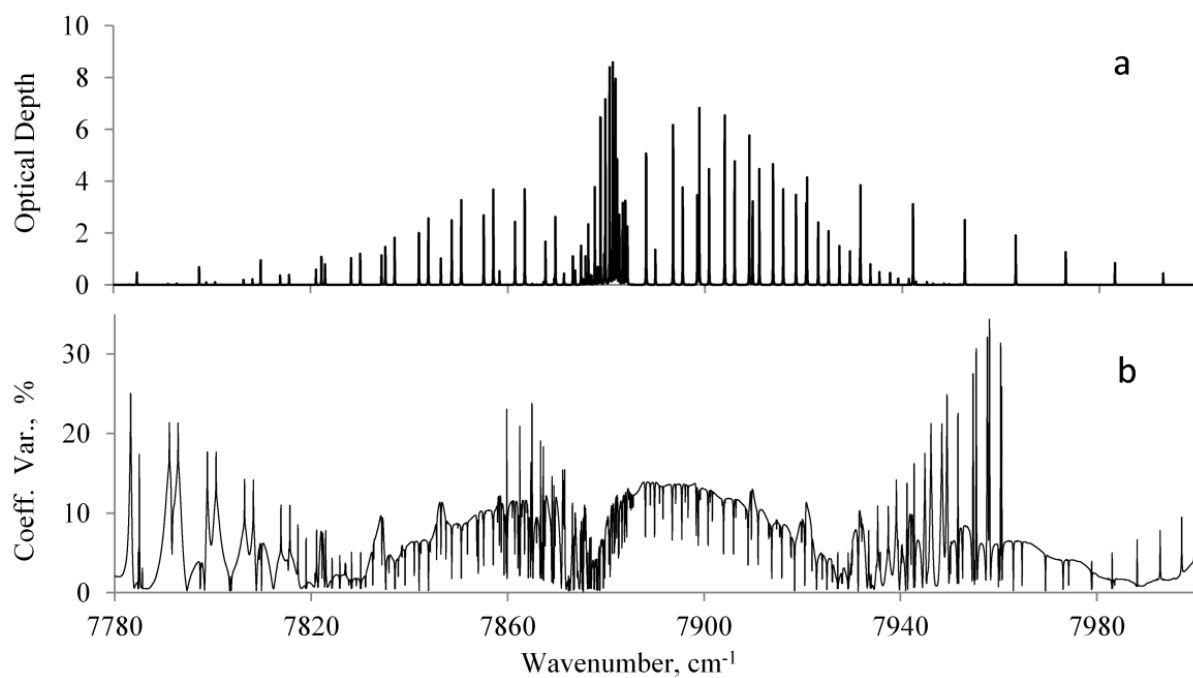


Fig 5. Total absorption spectrum for an 80km vertical path and US Standard atmospheric model (a) and the temperature induced error (b) for the 1.26-1.27 μm band of O_2 due to annual variations in atmospheric temperature for year 2009.

Of importance is the fact that the alternative CO₂ bands at 1.57 and 2.05 μm perform similarly providing a minimum temperature sensitivity of several percent in the least temperature sensitive regions.

We have also investigated the effect of temperature variations on the 1.26-1.27 μm and the A-Band of oxygen. The results of this analysis are summarized in Fig 4 and 5, showing the total transmission spectra for a vertical 80km path length (a) and the corresponding temperature induced uncertainty in percent (b). As can be seen from Fig 4b, the A-Band provides 2 regions of low temperature sensitivity at around 13060 and 13160 cm^{-1} , whereas the 1.26-1.27 μm region has 4 regions of low temperature sensitivity thus providing more options for wavelength selection. Namely the regions in the vicinity of 7820, 7875, 7930, and 7980 provide the lowest temperature sensitivity levels in the 1.26 – 1.27 μm band. Of importance is the fact that the temperature sensitivity performance is very similar in both bands of oxygen compared, reaching lowest uncertainties of several percent.

A closer comparison of temperature sensitivity analysis results for the 1.26-1.27 μm and A-Band Oxygen spectra is presented in Fig 6. As can be seen from Fig. 6b, the uncertainty induced due to temperature variations in the A-Band is about 7% for one of the candidate sensing wavelengths.^{11,12} The error in the 1.26-1.27 μm region corresponding to the location between the 2 closely located lines shown in Fig 5c reaches 10% which is slightly higher than that for the A-Band example. The results presented in Fig. 4, 5 and 6 indicate that the performance of the alternative bands of oxygen is about the same reaching its minimum temperature/pressure variation related error of 5 – 10% for the least temperature sensitive regions assuming no corrections for the known meteorological parameters. Taking into account the required accuracy of 0.3% in the final measurements for the sensing of CO₂ mixing ratios in the missions such as ASCENDS, additional corrections are required to eliminate the temperature dependence to the levels required to ensure the needed XCO₂ retrieval accuracy.

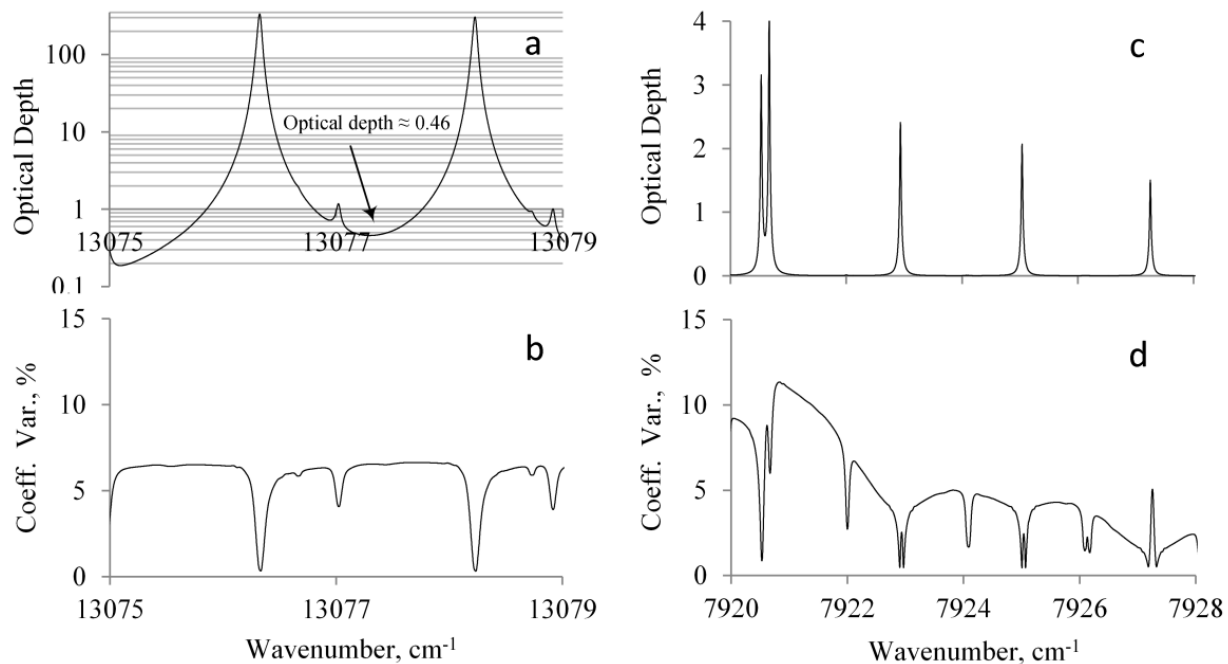


Fig 6 Comparison of temperature sensitivity levels for 2 candidate oxygen regions being investigated by several groups [Ref. 11, 12]. (a) and (c) are the transmission spectra for the lines for a vertical 80 km path obtained using US standard atmospheric model in the A-Band and the 1.26-1.27 micron bands of oxygen. (b) and (d) are the coefficients of variation due to temperature and pressure changes corresponding to spectra (a) and (c) respectively.

The results in Fig 6 suggest that generally the temperature induced error reaches its minimum at spectral line centers rapidly increasing as the wavelengths is moved away from the center of the line. As such, from the stand point of temperature sensitivity reductions, it is favorable to select wavelengths located more closely to the line center. Due to the above, Fig 6 comparison further suggests that lower temperature sensitivity levels are achievable in the 1.26-1.27 μm band compared to the A-Band due to the fact that measurement regions in the 1.26-1.27 micron band are located closer to the line centers to ensure high enough absorption levels. On the other hand, the A-Band consists of many strong oxygen lines imposing a requirement of significant displacements from the center of the lines to achieve favorable absorption levels.

The results shown for the single wavelength temperature sensitivity analysis suggest that the maximum temperature insensitivity levels that may be achieved in the A-Band and the 1.26-1.27 μm region of O_2 are about the same with uncertainties in the range of 5-10 percent, however the 1.26-1.27 μm band region has more low-temperature-sensitive regions and as such provides more options for possible low temperature sensitive O_2 line selections with fewer water vapor interferences. However, despite the larger number of temperature insensitive regions in the 1.26-1.27 μm band, it should be noted that the O_2 A-Band suffers fewer water vapor interferences.

3. TWO – WAVELENGTH (ON / OFF) TEMPERATURE AND PRESSURE SENSITIVITY ANALYSIS

In the previous section we have considered the temperature sensitivity analysis for a single wavelength case when no off-line correction is used. This section presents a sample differential absorption temperature and pressure sensitivity analysis to for a 1.57 μm band of CO_2 to illustrate the effect of the off-wavelength position onto the temperature induced uncertainty values assuming no atmospheric meteorological data corrections. Please refer to Ref. 8 for a description of the calculation methodology.

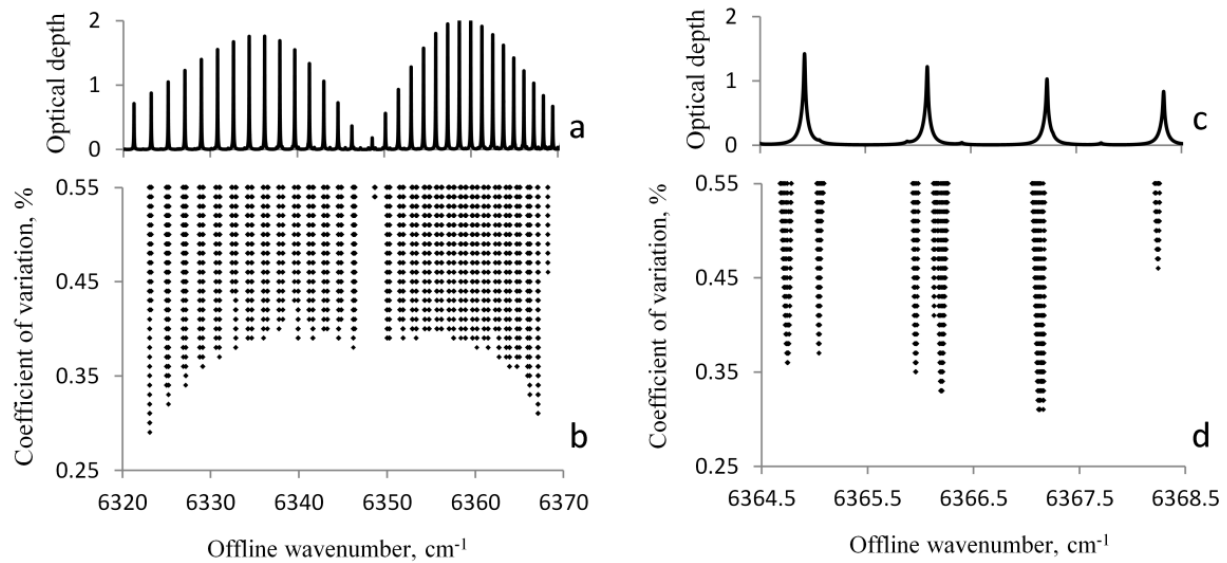


Fig 7. Intra-band differential absorption temperature sensitivity reduction as a function of off-line wavelength for a CO_2 online wavelength located within the $6364.722 - 6365.122 \text{ cm}^{-1}$ region (6364.922 cm^{-1} CO_2 line) and the off-line wavelength varied in the range of $6300\text{-}6380 \text{ cm}^{-1}$ with a differential on / off line optical depth value of 0.1 or larger.

Fig 7 illustrates the effect of various on- and off-line wavelength combinations on the resultant temperature sensitivity. Fig 7a shows a total transmission spectrum for a vertical path of 80km in the spectral range of $6320 - 6370$

cm^{-1} , the corresponding point plot of the coefficients of variation as a function of off-line wavelength is shown in Fig 7b. Fig 7b was obtained by maintaining the on-line wavelength within the 6364.922 cm^{-1} line of CO_2 ($6364.722 - 6365.122 \text{ cm}^{-1}$) and varying the off-line wavenumber in the $6300 - 6380 \text{ cm}^{-1}$ range. An additional condition on the on- and off-line wavelength combinations imposed in simulations was to maintain at least a minimum differential optical depth value of 0.1 or larger.¹³ Fig 7c and 7d are the plots corresponding to Fig 7a and 7b respectively for a shorter spectral region of $6364.5 - 6368.5 \text{ cm}^{-1}$ which better illustrates the effect of different off-line combinations selected. As can be seen from Fig 7b and 7d, better temperature insensitivity is achieved if the off-line wavelengths are selected within spectral lines different from that containing the on-line wavelength and having lower intensity than the on-line wavelength spectral line. This result suggests that the best temperature sensitivity cancelation is achieved when the on- and off-line wavelengths are selected within lines having close spectral parameters and are preferably equally spaced from the centers of the lines in terms of the spectral half width units. The combinations of on- and off- line wavelengths within the adjacent lines allows achieving at least the minimum on/off wavelength differential optical depth value by maintaining the location of on- and off- line wavelengths at half-width relative distances closer to each other resulting in better temperature sensitivity compensation.

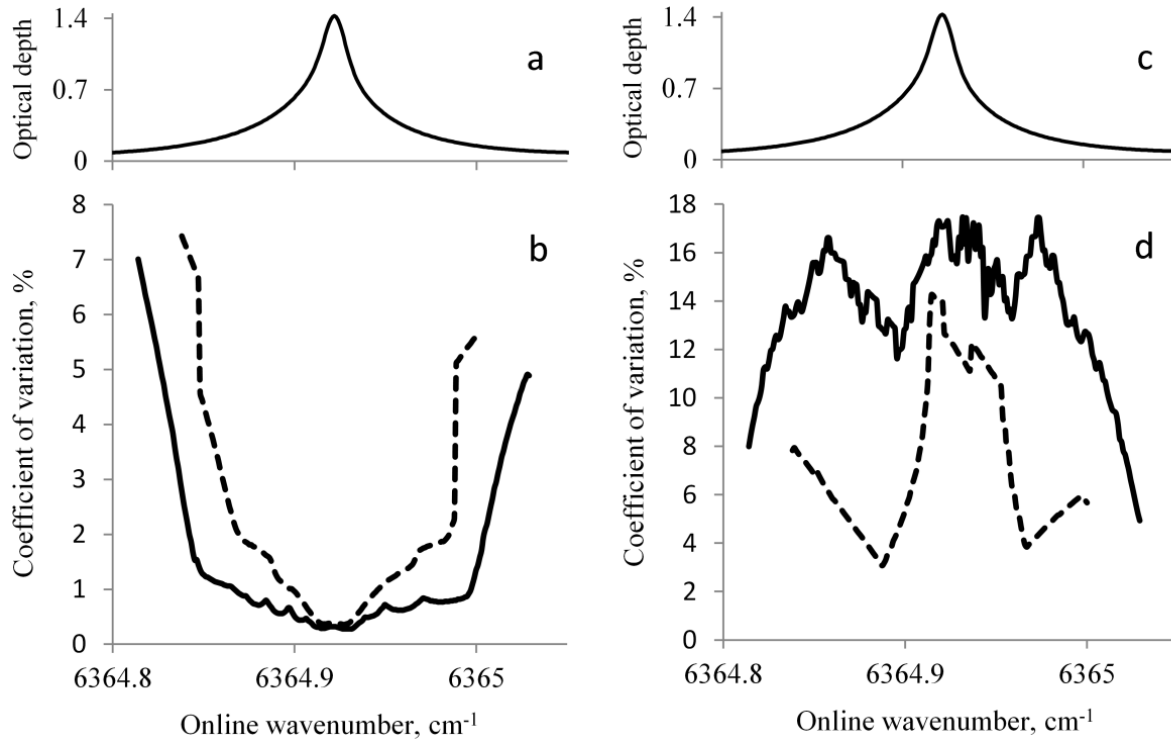


Fig. 8 Illustration of the effect of the off-line wavelength selection on the temperature sensitivity for an online wavelength located within the 6364.922 cm^{-1} spectral line ($6364.722 - 6365.122 \text{ cm}^{-1}$ region). Spectra in Fig 9a and 9c are the total optical depth for a vertical path of 80km, and the plots in Fig 9b and 9d show the minimum (b) and maximum (d) achievable coefficients of variation due to temperature changes as the off-line wavelength is changed within the $6364.722 - 6365.122 \text{ cm}^{-1}$ spectral region (dashed line) and when the off-line wavelength is changed in the $6300-6380 \text{ cm}^{-1}$ spectral region (solid line).

Fig 8 further illustrates the difference in the minimum and maximum temperature induced errors for a 6364.922 cm^{-1} spectral line of CO_2 as the off-line wavelength span is varied. The dashed curves have been obtained by keeping both the online and offline wavelengths within a single line wavenumber span of $6364.5 - 6368.5 \text{ cm}^{-1}$. The solid line on the other hand was obtained by maintaining the online wavelengths within the $6364.5 - 6368.5 \text{ cm}^{-1}$ spectral region and

varying the off-line wavelength over the entire spectral range of $6300 - 6380 \text{ cm}^{-1}$. As can be seen from Fig. 8b, selection of off-line wavelengths outside of a single absorption line used for the on-line wavelength (solid line) results in lower temperature sensitivity levels especially for spectral regions located further away from the line center.

This result further supports the assumption that better on-line / off-line wavelength matching is achieved resulting in higher temperature sensitivity cancellation levels for the off-lines selected within a line different from the one containing the measurement on-line wavelength. Additionally as can be seen from Fig 9d, with increased span of the off-line wavelength an incorrect selection of on- and off- line combinations may lead to higher temperature induced errors compared to the case when both the on- and off-line wavelengths located within the same spectral line.

The results of the temperature sensitivity analysis observations presented in this section have lead us to the alternative mixing ratio measurement approach called CoBRA described in.⁷⁻⁹

4. CONCLUSIONS

Regions of minimum temperature sensitivity were identified for all bands of CO_2 and O_2 currently under investigation for potential use in the sensing of CO_2 for missions such as ASCENDS. It is found that all bands perform about the same in terms of temperature induced uncertainties with the lowest relative uncertainty optical depth values of 1–5 % in the least temperature sensitive regions. Our results further show that the minimum temperature induced uncertainty for all spectral bands of CO_2 and O_2 being considered for the measurement of the carbon dioxide mixing ratios (XCO_2) typically has values of 5 – 10% for positions shifted from the line center which are favorable from the stand point of increased absorption near the surface.. These results provide useful information about the distribution and the magnitude of temperature induced uncertainties on an annual scale.

Measurements in the vicinity of line centers significantly reduce the temperature sensitivity but are unfavorable due to the stronger absorption at higher altitudes. These results confirm that additional temperature correction techniques are necessary to reduce the temperature sensitivities. This may be done by using the data from the Numerical Weather Prediction (NWP) models. Alternatively, we have suggested and are currently investigating CoBRA techniques for the measurement of the mixing ratios which hold potential for significant reductions in temperature and pressure uncertainties through proper matching of spectral line parameters⁷⁻⁹.

6. ACKNOWLEDGEMENTS

The authors acknowledge the support from the Earth Science and Technology Office (ESTO) and the NASA Postdoctoral Program (NPP).

7. REFERENCES

- [1] G. Ehret, C. Kiemle, M. Wirth, A. Amediek, A. Fix, S. Houweling,, "Space-borne remote sensing of CO_2 , CH_4 , and N_2O by integrated path differential absorption lidar: sensitivity analysis", *Appl. Phys. B*, **90**, pp. 593-608, (2008)
- [2] "Active Sensing of CO_2 Emissions over Nights, Days, and Seasons (ASCENDS) Mission", NASA Science Definition and Planning Workshop, July 23-25, 2008, Univ. of Michigan, Ann Arbor, MI, available at http://decadal.gsfc.nasa.gov/documents/12-30-08-ASCENDS_Workshop.pdf
- [3] D. Pluutau and N. S. Prasad, "Simulation framework to estimate the performance of CO_2 and O_2 sensing from space and airborne platforms for the ASCENDS mission requirements analysis", *Proc. SPIE* 8379, 83790K

- [4] D. Pliutau, N. Prasad, "Simulation studies for comparative evaluation of alternative spectral regions for the sensing of CO₂ and O₂ suitable for the ASCENDS Mission", Proc. SPIE **8513**, 851309 (SPIE Optics and Photonics 2012)
- [5] D. Pliutau, N. S. Prasad, "Integrated path differential absorption lidar optimizations based on pre-analyzed atmospheric data for ASCENDS mission applications", AGU Fall Meeting 2012, San Francisco, CA
- [6] D. Pliutau, N. Prasad, "Usage of data-encoded web maps with client side color rendering for combined data access, visualization and modeling purposes", SPIE Defense Security and sensing 2013, Baltimore, MD, 29 April - 3 May, 2013
- [7] D. Pliutau, N. Prasad, "Cross-band Relative Absorption Technique for Molecular Mixing Ratio Determination", submitted to CLEO 2013, San Jose CA, 9 – 14 June, 2013
- [8] D. Pliutau, N. Prasad, "Semi-empirical validation of the cross-band relative absorption technique for the measurement of molecular mixing ratios", SPIE Defense Security and sensing 2013, Baltimore, MD, 29 April - 3 May, 2013
- [9] N. Prasad, D. Pliutau, "Cross-band relative absorption technique for the measurement of molecular mixing ratios", (submitted to Optics Express).
- [10] Robert T. Menzies, and David M. Tratt, "Differential laser absorption spectrometry for global profiling of tropospheric carbon dioxide: selection of optimum sounding frequencies for high-precision measurements", Applied Optics, Vol 42, No. 33, pp. 6569-6577, (2003)
- [11] Susan Kooi, Jianping Mao, James B. Abshire, Edward V. Browell, Clark J. Weaver, Stephen R. Kawa, "Analysis of Vertical Weighting functions for lidar measurements of atmospheric CO₂ and O₂", **A21D**, 2011 AGU Fall Meeting, San Francisco, CA, 2011.
- [12] H. Riris, M. Rodriguez, G. Allan, W. E. Hasselbrack, M. A. Stephen, and J. B. Abshire, "Airborne LIDAR Measurements of Atmospheric Pressure Made Using the Oxygen A-band," in Lasers, Sources, and Related Photonic Devices, OSA Technical Digest (CD) (Optical Society of America, 2012), paper LT2B.5
- [13] Ellis E. Remsberg and Larry L. Gordley, "Analysis of differential absorption lidar from the space shuttle," Appl. Opt. **17**, 624-630 (1978)